Electron Diffraction and the Crystal Structure of Graphite

[redacted]

Abstract

The electron diffraction The wave-particle duality of an electron was observed. The interplanar distances d_{110} and d_{100} of graphite were derived geometrically and experimentally. By analyzing the equilateral triangle unit cell, d_{110} and d_{100} were 123 and 213 pm. These same distances were derived experimentally through electron diffraction by using Bragg's Law and De Broglie's equation, where d_{110} and d_{100} were calculated as 95 and 166 pm. While these pairs of values differ, their ratios (d_{100}/d_{110}) were similar at 1.73 and 1.75 for the geometrical and experimental approach respectively. The two ratios were similar to the accepted value of $\sqrt{3} \approx 1.73$.

Introduction

Electron Diffraction examines the wave-like behavior of electrons, which was first postulated by Louis de Broglie in 1924. Every particle has a wavelength, λ proportional to the inverse of its momentum:

$$\lambda = h/p \quad (1)$$

If electrons exhibit wave-like properties, then they could be diffracted through gratings with orders of magnitude equal to that of its De Broglie wavelength: these gratings are crystalline lattices. The experiment was first conducted by Davison and Germer at Bell Labs in 1927. Electrons incident on crystalline nickel produced diffraction peaks [1]. In order to create a beam of electrons, a potential is applied by a cathode ray tube. An expression for momentum is derived from the Kinetic energy gained by the electron in the electric field.

$$K = \frac{1}{2} m_e v^2 = \frac{p^2}{2m_e} = U_a e \Rightarrow p = \sqrt{2m_e U_a e} \quad (2)$$

Combining equations (1) and (2), the principle relationship for the lab is derived:

$$\lambda = h/\sqrt{2mU_a e} \quad (3)$$

Planck's Constant **Mass of Electron** **Fundamental Charge**

$$h: 6.626 \times 10^{-34} Js, \quad m_e = 9.109 \times 10^{-31} kg, \quad e = 1.602 \times 10^{-19} C$$

For crystalline structures, like graphite and nickel, there are infinite families of planes with corresponding spacings. Assuming every plane acts as a mirror, the diffraction angle traveled by the wave-like electron is determined by Bragg's Law:

$$2d \sin(\theta) = n\lambda \quad (4)$$

Where d is the spacing between planes and n is the order of the diffraction. Observe figure 1 for a geometric interpretation.

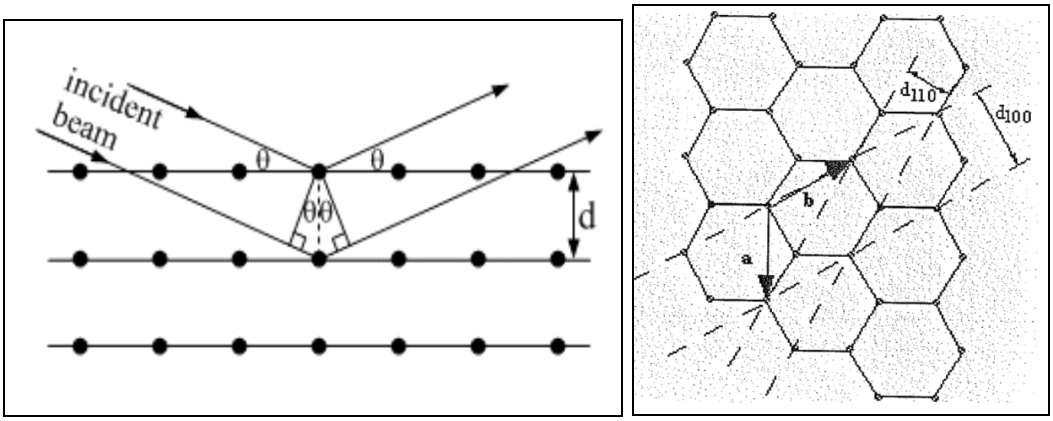


Figure 1: (Right) Bragg's Law for two parallel planes of atoms. Incident beams of electrons are in phase (produce a bright peak) when they strike an angle θ relative to the planes with spacing d between. (Left) d_{100} and d_{110} are the distances between lattice planes of graphite

Powdered graphite planes are used as diffraction gratings. Carbon atoms in graphite are sp^2 hybridized, and form hexagonal planes that are weakly bonded to one another (through delocalized π bonds). The electron beam is spread out and diffracts when incident on the graphite sample. The electrons produce a diffraction pattern according to which crystalline plane they diffract off. Figure 1 shows planes (100) and (110) with different spacings d_{100} and d_{110}. These two spacings will produce two distinct rings with order n = 1 and 2. We also note that the ratio $d_{100}/d_{110} = \sqrt{3}$. The diffraction cones have half angles governed by:

$$\tan(2\theta_{Bragg}) \approx r/2R \quad (6)$$

r is the radius of the diffraction pattern and R is the radius of the tube. Through the small angle approximation, we approximate $\sin 2\theta \approx \tan 2\theta \approx 2\sin\theta$.
Combining (4) and (6) along with the above approximation:

$$rd/2R = n\lambda \rightarrow r = \frac{2R}{d}n\lambda \quad (7)$$

Finally, combining (7) with (3):

$$r = \frac{2R}{d}n\frac{h}{\sqrt{2meU_a}} \quad (8)$$

Procedure

This section describes the apparatus used, a list of equipment, and the steps taken to gather data.

Description of the Apparatus + List of equipment:

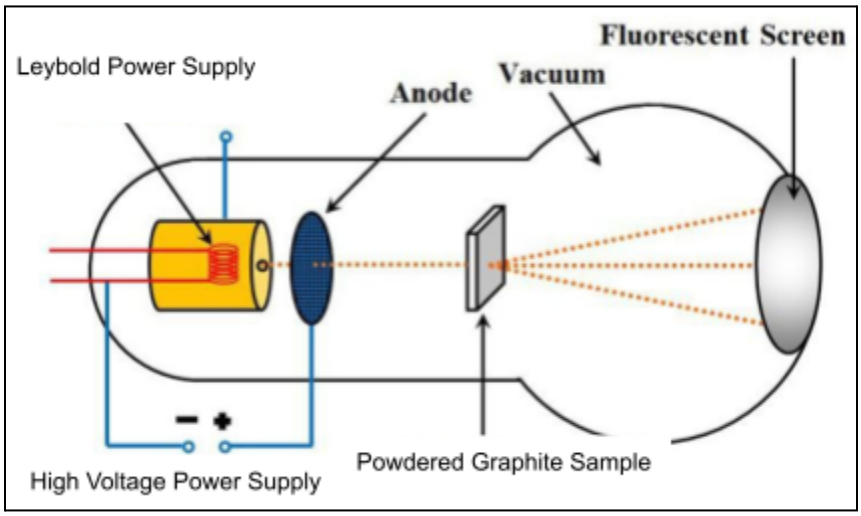


Figure 2: Diagram of the electron diffraction apparatus. Note that a vacuum is pulled such that the electrons do not interact with air particles. [Toppr]

1. **Power Supply Unit (0-20V):** Cathode
2. **High Power Supply Unit (0 kV - 5.0 kV ±0.05 kV):** Anode
   Heats up a metallic filament that emits electrons.
3. **Electron Diffraction Tube: (R = 65 mm)**
   An electron gun emits a beam of electrons that is accelerated towards a graphite sample. A vacuum is pulled throughout so that the electrons' path is straight.
4. **Graphite Sample:**
   Graphite, being sp^2 hybridized, comprises 2D sheets. When the bonds between sheets are broken, their orientation is randomized. Macroscopically this occurs when the graphite sample is powder or poly-crystal.
5. **Fluorescent Screen:**
   The fluorescent screen lights up a green color when the waves (of electrons) are incident upon it. The rings can then be measured using calipers.
6. **Plastic vernier calipers: (± 0.5 mm)**
   Calipers are used to measure the radius of the interference rings.

Experimental Procedure:

1. Turn on the Leybold power supply, wait 30 seconds for the circuit to "warm up"

2. Turn on the high voltage supply and wait 60 more seconds.
3. Increase the voltage to 2.6 kV and increment the voltage in steps of 0.2 kV.
4. For every increment, two rings should appear on the fluorescent screen
5. Using the calipers, measure both the inner and diameters of the smaller and larger rings. Thus for each step in voltage, there should be 4 data points. See measurement techniques for more details.
6. Repeat steps 3 to 5 once again. A different student should record the measurements the second time around.

Results

Voltage (±0.05kV)	Radius of Inner Ring (±0.5mm)	Radius of Outer Ring (±0.5mm)	Δ Radii (mm)	Wavelength (pm)	Δ Wavelength (±pm)
2.6	21.50	36.25	0.18	24.05	2.3 E-01
2.8	19.50	33.50	0.18	23.17	2.1 E-01
3.0	18.38	31.75	0.18	22.39	1.9 E-01
3.2	17.25	30.50	0.18	21.68	1.7E-01
3.4	16.50	29.00	0.18	21.03	1.6 E-01
3.6	15.75	27.25	0.18	20.44	1.4 E-01
3.8	15.00	26.50	0.18	19.89	1.3 E-01
4.0	14.50	25.00	0.18	19.39	1.2 E-01
4.2	14.00	24.00	0.18	18.95	1.1 E-01
4.4	13.25	23.75	0.18	18.49	1.1 E-01
4.6	13.25	23.25	0.18	18.08	1.1 E-01
4.8	12.50	22.50	0.18	17.70	9 E-02
5.0	12.25	21.25	0.18	17.34	9 E-02

Figure 3: Data of inner and outer average diffraction radii along with calculated and instrumental uncertainties.

Both the inner and outer diameter were measured for each ring, and then divided by two to get the radii of the interference rings. The inner and outer radii in figure 3 are the averages of two trials measured at the same voltage intervals. Wavelength calculations were made using equation (3). Wavelength uncertainty was calculated with the following uncertainty propagation.

$$\Delta\lambda = \sqrt{\left(\frac{\partial\lambda}{\partial U}\Delta U_A\right)^2} \rightarrow \Delta\lambda = \sqrt{\left(\frac{\partial}{\partial U_A}\left(\frac{h}{\sqrt{2meU_A}}\right)\Delta U_A\right)^2}$$

$$\Delta\lambda = \sqrt{\left(-0.5\frac{2meh}{(2meU_A)^{3/2}}\Delta U_A\right)^2}$$

Uncertainties of the radii refer to the reading uncertainty of the vernier caliper and do not account for human measurement errors.

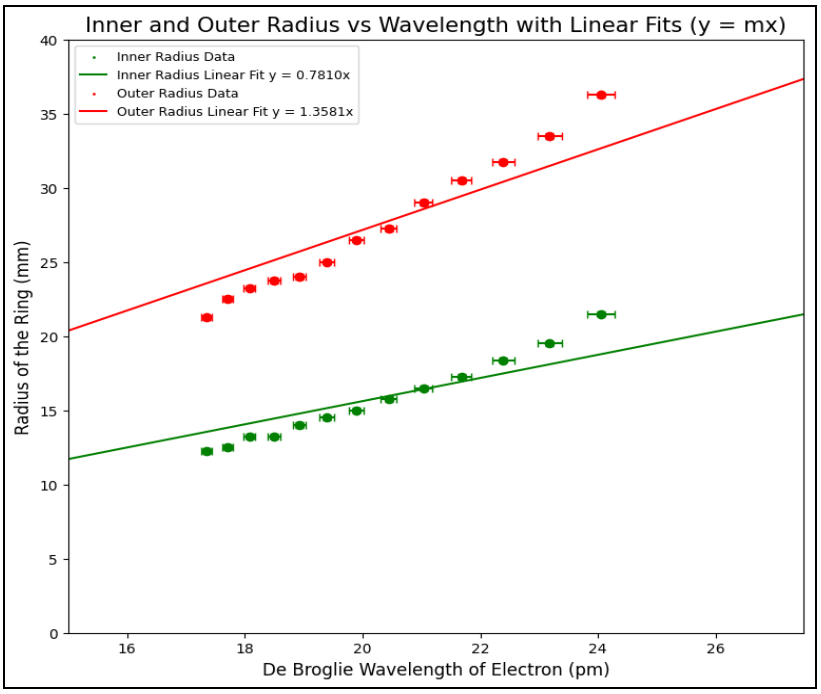
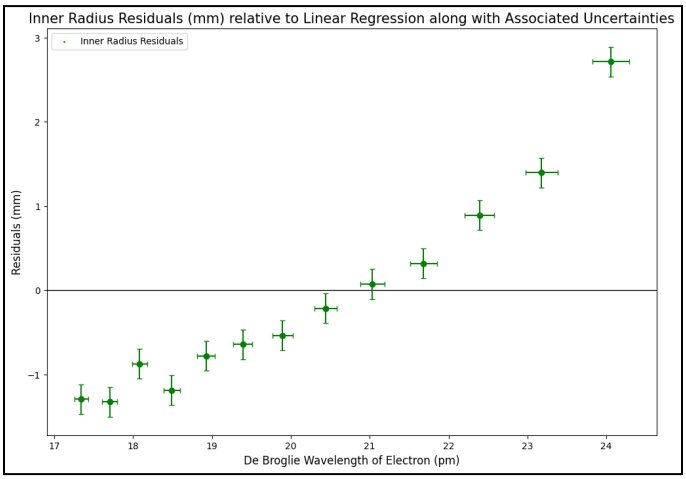


Figure 4: Linear fit of radii fit against wavelengths where m_1 and m_2 represent the slope of the inner (order n = 1, χ^2 = 0.887) and outer (order n = 2, χ^2 = 0.852) radii respectively.



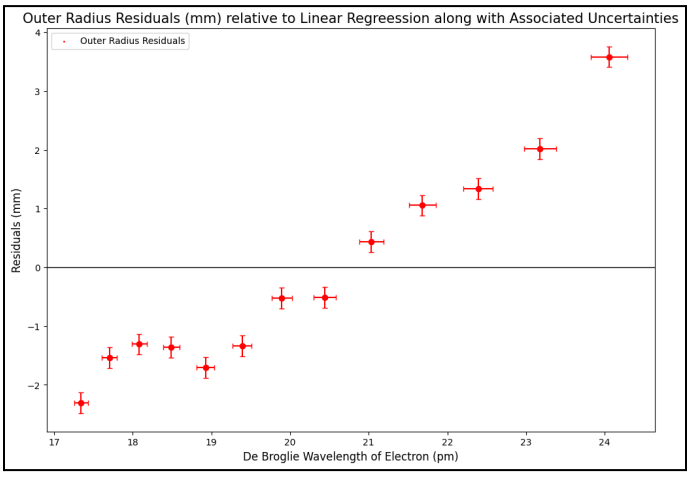


Figure 5: Residuals of linear regression.

Figure 4 shows the linear relationship between diffraction radii and wavelength. By equation (3), wavelength is inversely proportional to the square root of anode voltage. Equation (8) demonstrates the linear proportionality of radii to wavelength. Therefore, the linear fit of figure 4, as supported by the χ^2 values of 0.887 and 0.852, support the dependence of diffraction radii on anode voltage. The uncertainty for slope m_1 and m_2 were calculated with Linest to be 0.027, 0.046, respectively.

Analysis

This section examines the particle-wave nature of electrons, graphite crystal structure, and sources of potential error.

Particle-Wave Duality of Electrons:

At higher voltages, flickering of the screen at the center of the rings was observed. The flickering may be attributed to electrons from the beam that are not diffracted by the graphite sample and instead pass straight through. The electrons that pass through the sample still exhibit their particle-like behavior as they strike the fluorescent screen along the same path as the beam of electrons. Moreover, the tube is evacuated to limit the probability of the electron particle colliding with air molecules.

As the electrons strike the sample, they are scattered throughout the atomic structure. According to the planes they hit, they will either interfere constructively or destructively with each other through the phenomena of diffraction. The constructive interference causes the fluorescent screen to light up, while the destructive interference corresponds to dark spots on the screen. This is referred to as a diffraction pattern. Diffraction patterns are properties of waves. For example, a coherent beam of light incident on thin slits (diffraction grating), causes constructive (bright fringes) and destructive interference (dark fringes) to occur. In a similar fashion, the graphite sample acts as a diffraction grating for the beam of electrons. The "slits" are effectively the distances between neighboring planes/atoms.

Interplanar d-Spacing:

From equation (7), we have a proportional relationship between the ring radii and the wavelength. Figure (y = mx) shows the relationship received from the data. The slope, therefore, corresponds to:

$$r = \frac{2R}{d} n\lambda \rightarrow r = m_1 \lambda$$

$$r = \frac{2R}{d} n\lambda \rightarrow r = m_2 \lambda$$

where m_1 and m_2 represent the slope of the inner (order n = 1) and outer (order n = 2) radii functions respectively. Using $m_1 = 0.781$ and $m_2 = 1.358$, spacing of the d_{100} plane is calculated as 166 pm ± 0.027 and spacing of the d_{110} plane is calculated as 95.6 pm ± 0.046. The ratio between planes d_{100} and d_{110} is 166 pm/95.6 pm = 1.74 which strongly agrees with the theoretical ratio of $\sqrt{3}$ in equation (5). The fractional uncertainty is negligible in this calculation.

Crystal Structure of Graphite:
Assuming the unit cell is an equilateral triangle, the volume of the unit cell can be found using the following equation:

$$v = \frac{n \cdot W}{\rho \cdot N_A} = \frac{3\sqrt{3}}{4} x^2 h \quad (9)$$

Where n = 1, the number of atoms in a unit cell, W = 12 g/mol is the atomic weight of carbon, ρ = 2.25 g/cm^3 is the density of graphite, h = 3.4 Å is the average separation between layers, and x is the distance between nearest neighboring atoms. Rearranging equation (9), x can is calculated as 1.42 Å. Due to the geometry of the plane and the hexagonal structure of carbon planes, as shown in figure 1:

$$d_{110} = x sin30^\circ \quad \text{and} \quad d_{100} = x + x sin30^\circ$$

Then d_{110} = 123 pm and d_{100} = 213 pm. While this does not agree with our previous calculations of d-spacing, the ratio of $\frac{213}{123} = 1.73$ is consistent with equation (5). This suggests that there may have been systematic errors in data collection, such as neglecting the curvature of the tube face.

Sources of Error:
The curvature of the tube face and the thickness of the glass was neglected when measuring diameter which results in smaller diameter values. This systematic error impacts the uncertainty in measurements of the outer ring radii greater than the inner ring radii because of the additional curvature. This can be observed by comparing the magnitude of total residuals of the linear fit in figure 5. One way to reduce this error is to interpolate the measurement. Another source of potential error was due to manual, by hand, data collection methods. Two trials were averaged in an attempt to mitigate related errors. The small angle approximation for diffraction angle and tube curvature in equation (8) may also be a source of potential error. At θ = 10, the largest fractional error for both small angle approximations is around 2%, and increases to 6% when θ = 20. The electron beam may not be perfectly aligned with the carbon sample, and depending on the severity, small angle approximations may have ignored potential error.

The equations provided in this report use the non-relativistic definition of momentum in its derivations, which is inaccurate since electrons are accelerated through the cathode tube at a speed where laws of relativity become significant. The following equation can be derived using Einstein's equations of relativity.

$$\lambda_r = \frac{h}{\sqrt{2mk(1+\frac{k}{2mc^2})}}$$

Taking the ratio of the classical wavelength equation, equation (3), and the relativistic wavelength equation:

$$\frac{\lambda_c}{\lambda_r} = \sqrt{1 + \frac{k}{2mc^2}}$$

Thus, if the kinetic energy is significantly less than mc^2 the classical de Broglie wavelength equation yields a negligible error. Using equation (2), k at 5.0 kV is calculated to be 8.01×10^{-16} and mc^2 is 8.20×10^{-14}, resulting in an error of 0.2%. This indicates that the classical equation for De Broglie wavelength has negligible error within the range of anode voltages in this experiment.

Conclusion

The wave-particle nature of electrons were observed. The linear relationship between wavelength and diffraction radii were confirmed. From the diffraction patterns the interplanar spacing for a diffraction order of n =1 and n= 2 was calculated to be 123 pm and 213 pm, respectively. While these values did not align with the values found using the geometry of the hexagonal structure of the carbon plane, both methods yielded a d_{100} to d_{110} ratio similar to the theoretical ratio of $\sqrt{3}$. This error is most likely systematic and could be addressed by using more accurate data collection methods that involve taking the curvature of the tube face into account. Further improvements could be made by collecting more data points so that the linear fit is more precisely expressed or performing extensive error propagation to better understand the validity of calculated results and values.

References

[1] IWantToLearn. “Relativistic Calculations for De-Broglie Wavelength.” *Physics Forums: Science Discussion, Homework Help, Articles*, Physics Forums: Science Discussion, Homework Help, Articles, 13 Nov. 2015, www.physicsforums.com/threads/relativistic-calculations-for-de-broglie-wavelength.842731/.

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